GENERALIZED SIMULATED ANNEALING

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Abstract

We propose a new stochastic algorithm (*generalized simulated annealing*) for computationally finding the *global* minimum of a given (not necessarily convex) energy/cost function defined in a continuous D-dimensional space. This algorithm recovers, as particular cases, the so called *classical* ("Boltzmann machine") and *fast* ("Cauchy machine") simulated annealings, and can be quicker than both.

Key-words: Simulated annealing; Nonconvex optimization; Gradient descent; Generalized Statistical Mechanics.

1 INTRODUCTION

The central step of an enormous variety of problems (in Physics, Chemistry, Statistics, Neural Networks, Engineering, Economics) is the minimization of an appropriate energy/cost function defined in a D-dimensional continuous space ($\vec{x} \in \mathbb{R}^D$). If the energy is *convex* (single minimum), any gradient descent method easily solves the problem. But if the energy is *nonconvex* (multiple extrema) the solution requires more sophisticated methods, since a gradient descent procedure could easily trap the system in a *local* minimum (instead of one of the *global* minima we are looking for). This sophistication must necessarily involve possible "hill climbings" (for detrapping from local minima), and can be heavily computer-time-consuming. Consequently, various algorithmic strategies have been developed along the years for making this important problem increasingly tractable. One of the generically most efficient (hence popular) methods is *simulated annealing*, to which this paper is dedicated. In this technique, one or more artificial temperatures are introduced and gradually cooled, in complete analogy with the well known annealing technique frequently used in Metallurgy for making a molten metal to reach its crystalline state (*global* minimum of the thermodynamical energy). This artificial temperature (or set of temperatures) acts as a *source of stochasticity*, extremely convenient for eventually detrapping from local minima. Near the end of the process, the system hopefully is inside the attractive basin of the *global* minimum (or in one of the global minima, if more than one exists, i.e., if there is *degeneracy*), the temperature is practically zero, and the procedure asymptotically becomes a gradient descent one. The challenge is to cool the temperature the quickest we can *but* still having the guarantee that no definite trapping in *any* local minimum will occur. More precisely speaking, we search for the *quickest annealing* (i.e., in some sense approaching a *quenching*) which preserves the probability of ending in a global minimum being equal to one. The first nontrivial solution along this line was provided in 1983 by Kirkpatrick et al [1] for classical systems, and was extended in 1986 by Ceperley and Alder [2] for quantum systems. It strictly follows quasi-equilibrium Boltzmann-Gibbs statistics. The system "tries" to visit, according to a *visiting distribution* assumed to be *Gaussian* (i.e., a *local* search distribution) in the neighborhood of its actual state $\vec{x}$. The jump is *always accepted* if it is down hill (of the energy/cost funtion); if it is hill climbing, it *might be accepted* according to an *acceptance proba-*

bility assumed to be the canonical-ensemble Boltzmann-Gibbs one. Geman and Geman [3] showed, for the classical case, that a necessary and sufficient condition for having probability one of ending in a global minimum is that the temperature decreases *logarithmically* with time. This algorithm is sometimes referred to as *classical simulated annealing* (CSA) or *Boltzmann machine*. We easily recognize that, if instead of decreasing, the temperature was maintained fixed, this procedure precisely is the well known Metropolis et al [4] one for simulating thermostatistical equilibrium.

The next interesting step along the present line was Szu's 1987 proposal [5] of using a Cauchy-Lorentz visiting distribution, instead of the Gaussian one. This is a *semi-local* search distribution: the jumps are frequently local, but can occasionally be quite long (in fact, this is a Lévy-flight-like distribution). The acceptance algorithm remains the same as before. As Szu and Hartley showed, the cooling can now be much faster (the temperature is now allowed to decrease like the *inverse* of time), which makes the entire procedure quite more efficient. This algorithm is referred to as *fast simulated annealing* (FSA) or *Cauchy machine*.

The goal of the present work is to generalize *both* annealings within an unified picture which is inspired in the recently Generalized Statistical Mechanics [6, 7] (see also [8, 9]), with the supplementary bonus of providing an algorithm which is *even quicker* than that of Szu's. In Section 2, we briefly review this generalized thermostatistics, describe the optimization algorithm and prove that, if the cooling rithm is appropriate, the probability of ending in a global minimum equals one. In Section 3, we numerically discuss a simple $D = 1$ example. Finally, we conclude in Section 4.

2 GENERALIZED SIMULATED ANNEALING (GSA)

Inspired by multifractals, one of us proposed [6] a generalized entropy S_q as follows

$$S_q = k \, \frac{1 - \sum_i p_i^q}{q - 1} \qquad (q \in \mathbb{R}) \tag{1}$$

where $\{p_i\}$ are the probabilities of the microscopic configurations and k is a conventional positive constant. In the $q \to 1$ limit, S_q recovers the well known Shannon expression $-k_B\sum_i p_i \ln p_i$. Optimization of this entropy for the canonical ensemble yields

$$p_i = \frac{[1-\beta(1-q)E_i]^{\frac{1}{1-q}}}{Z_q} \tag{2}$$

with

$$Z_q \equiv \sum_i \, [1-\beta(1-q)E_i]^{\frac{1}{1-q}} \tag{3}$$

where $\beta \equiv 1/kT$ is a Lagrange parameter, and $\{E_i\}$ is the energy spectrum. We immediately verify that, in the $q \to 1$ limit, we recover Boltzmann-Gibbs statistics, namely $p_i = \exp(-\beta E_i)/Z_1$ with $Z_1 \equiv \sum_i \exp(-\beta E_i)$.

Let us now focus the *acceptance probability* $P_{q_A}(\vec{x}_t \to \vec{x}_{t+1})$, where t is the discrete time ($t = 1, 2, 3, \cdots$) corresponding to the computer iterations. For the Boltzmann machine ($q_A = 1$) we have, for example, the Metropolis algorithm [4] :

$$P_1(\vec{x}_t \to \vec{x}_{t+1}) = \begin{cases} 1 & \text{if } E(\vec{x}_{t+1}) < E(\vec{x}_t) \\ e^{[E(\vec{x}_t)-E(\vec{x}_{t+1})]/T_1^A(t)} & \text{if } E(\vec{x}_{t+1}) \geq E(\vec{x}_t) \end{cases} \tag{4}$$

where $T_1^A(t)$ is the $q_A = 1$ *acceptance temperature* at time t ($k = 1$ from now on). We see that $T_1^A(t) = +0$ implies $P_1 = 1$ if $E(\vec{x}_{t+1}) < E(\vec{x}_t)$, and $P_1 = 0$ if $E(\vec{x}_{t+1}) \geq E(\vec{x}_t)$. These limits are important for the asymptotic stabilization of the annealing process,and we will require them to be satisfied by the generalized form. Eq.(4) satisfies detailed balance. A generalization of Eq.(4) that also satisfies the detailed balance condition, and asymptotically generates states distributed according to Eq.(2), must involve the ratio of terms of the form $1-\beta(1-q)E$. Nevertheless, we could not find a generalization along this line which satisfies the $T = 0$ limits mentioned above. Instead, we worked with a form that generalizes Eq.(4), satisfies the limits at $T = 0$, and goes to an equilibrium distribution, although generically different from that of Eq.(2). This generalized acceptance probability reads:

$$P_{q_A}(\vec{x}_t \to \vec{x}_{t+1}) = \begin{cases} 1 & \text{if } E(\vec{x}_{t+1}) < E(\vec{x}_t) \\ \frac{1}{\left[1+(q_A-1)(E(\vec{x}_{t+1})-E(\vec{x}_t))/T_{q_A}^A\right]^{\frac{1}{q_A-1}}} & \text{if } E(\vec{x}_{t+1}) \geq E(\vec{x}_t) \end{cases} \tag{5}$$

Although it is possible to work under generic conditions, for simplicity we shall assume here that $E(\vec{x}) \geq 0$ $(\forall \vec{x})$. Moreover, we shall assume that $q_A \geq 1$, so $T^A_{q_A}(t)$ can decrease *down to zero* without any type of singularities. Within these hyphothesis, $P_{q_A} \in [0,1]$ $(\forall q_A)$, and, for $T^A_{q_A}(t)$ decreasing from infinity to zero, P_{q_A} monotonically varies from 1 to 0 if $E(\vec{x}_{t+1}) \geq E(\vec{x}_t)$, and equals 1 whenever $E(\vec{x}_{t+1}) < E(\vec{x}_t)$.

We can now focus the $\vec{x}_t \to \vec{x}_{t+1}$ isotropic *visiting distribution* $g_{q_V}(\Delta x_t)$ where $\Delta x_t \equiv (\vec{x}_{t+1} - \vec{x}_t)$. It satisfies

$$\Omega_D \int_0^\infty d\rho \ \rho^{D-1} g_{q_V}(\rho) = 1 \tag{6}$$

where $\Omega_D \equiv D\Pi^{D/2}/\Gamma\left(\frac{D}{2}+1\right)$ is the D-dimensional complete solid angle. For the Boltzmann machine ($q_V = 1$) we have [1, 5]

$$g_1(\Delta x_t) \propto \exp\left[-\frac{(\Delta x_t)^2}{T^V_1(t)}\right] \tag{7}$$

where $T^V_1(t)$ is the $q_V = 1$ *visiting temperature* at time t. Using condition (6) we obtain

$$g_1(\Delta x_t) = \frac{e^{-\frac{(\Delta x_t)^2}{T^V_1(t)}}}{[\pi \ T^V_1(t)]^{D/2}} \tag{8}$$

For the Cauchy machine ($q_V = 2$) we have [5]

$$g_2(\Delta x_t) \propto \frac{T^V_2(t)}{\{[T^V_2(t)]^2 + (\Delta x_t)^2\}^{\frac{D+1}{2}}} \tag{9}$$

where $T^V_2(t)$ is the $q_V = 2$ *visiting temperature* at time t. The functional form of Eq. (9) is the D-dimensional Fourier transform of $\exp\{-T^V_2(t)|\vec{y}|\}$ (see [5]). Using condition (6) we obtain

$$g_2(\Delta x_t) = \frac{\Gamma(\frac{D+1}{2})}{\pi^{\frac{D+1}{2}}} \frac{T^V_2(t)}{\{[T^V_2(t)]^2 + (\Delta x_t)^2\}^{\frac{D+1}{2}}} \tag{10}$$

Within the present scheme, a natural proposal for unifying (8) and (10) is

$$g_{q_V}(\Delta x_t) = c\frac{[T^V_{q_V}(t)]^d}{\{[T^V_{q_V}(t)]^e + (q_V - 1)b(\Delta x_t)^2\}^{\frac{a}{q_V-1}}} \tag{11}$$

where a, b, c, d and e are (q_V, D)-dependent pure numbers to be determined. Using condition (6) and recalling that Δx_t may carry dimensions (e.g, [length]) we immediately establish that

$$d = e\frac{2a - D(q_V - 1)}{2(q_V - 1)} \qquad (\forall q_V, \forall D) \tag{12}$$

To further decrease the number of independent pure numbers to be determined, let us address a central point, namely the fact that the method has to guarantee that, at the $t \to \infty$ limit, the system must be at a *global* minimum. For this to occur (see [5] and references therein) the state visiting must be *"infinite often in time (iot)"*, which indeed occurs if $\sum_{t=t_0}^{\infty} g_{q_V}(\Delta x_{t_0})$ *diverges* for fixed Δx_{t_0} with $t_0 >> 1$. Under these conditions we have that

$$\sum_{t=t_0}^{\infty} g_{q_V}(\Delta x_{t_0}) \propto \sum_{t=t_0}^{\infty} [T_{q_V}^V(t)]^d \tag{13}$$

We know [5] that, for arbitrary D, $T_1^V(t) = T_1^V(1)\ln 2/\ln(1+t)$ and $T_2^V(t) = T_2^V(1)/t$, which are conveniently unified with

$$\begin{aligned} T_{q_V}^V(t) &= T_{q_V}(1)\frac{2^{q_V-1}-1}{(1+t)^{q_V-1}-1} && (14) \\ &\sim T_{q_V}(1)\frac{2^{q_V-1}-1}{t^{q_V-1}} \qquad (t \to \infty) && (14') \end{aligned}$$

Replacing (14') into Eq. (13) we obtain

$$\sum_{t=t_0}^{\infty} g_{q_V}(\Delta x_{t_0}) \propto \sum_{t=t_0}^{\infty} \frac{1}{t^{(q_V-1)d}} \tag{15}$$

For arbitrary D and $q_V = 1, 2$ it is [5] $(q_V - 1)d = 1$. We assume, for simplicity, that the same holds $\forall q_V$, hence

$$d = \frac{1}{q_V - 1} \qquad (\forall q_V, \forall D) \tag{16}$$

consequently the series (15) is the *harmonic* one, hence *diverges* (logarithmically) as desired. If we use Eqs. (12) and (16) into (11) we obtain

$$g_{q_V}(\Delta x_t) = c\frac{[T_{q_V}^V(t)]^{\frac{-D}{2a-D(q_V-1)}}}{\left\{1 + (q_V - 1)b\frac{(\Delta x_t)^2}{[T_{q_V}^V(t)]^{\frac{2}{2a-D(q_V-1)}}}\right\}^{\frac{a}{q_V-1}}} \tag{17}$$

For $q_V = 1$, Eq. (17) must recover Eq. (8), hence $b = 1$ and $a = 1$ (for arbitrary D). For $q_V = 2$, Eq. (17) must recover Eq. (10), hence $b = 1$ and $a = \frac{D+1}{2}$ (for arbitrary D). For simplicity we assume

$$b = 1 \qquad (\forall q_V,\ \forall D) \tag{18}$$

Finally, condition (6) univocally determines the normalizing pure number c as a function of the rest of the free parameters. Using this and Eq. (18) into Eq. (17) yields

$$g_{q_V}(\Delta x_t) = \left(\frac{q_V - 1}{\pi}\right)^{D/2} \frac{\Gamma\left(\frac{a}{q_V-1}\right)}{\Gamma\left(\frac{a}{q_V-1} - \frac{D}{2}\right)} \frac{[T^V_{q_V}]^{-\frac{D}{2a - D(q_V-1)}}}{\left\{1 + (q_V - 1)\frac{(\Delta x_t)^2}{[T^V_{q_V}(t)]^{\frac{2}{2a-D(q_V-1)}}}\right\}^{\frac{a}{q_V-1}}} \tag{19}$$

where *only one* undetermined pure number (namely $a(q_V, D)$) is now left. It satisfies, as already mentioned, $a(1, D) = 1$ and $a(2, D) = (D + 1)/2$. Although more general forms are possible, we shall adopt the simplest q_V-dependence, namely a linear interpolation, hence

$$a = 1 + \frac{D-1}{2}\,(q_V - 1) \qquad (\forall q_V,\ \forall D) \tag{20}$$

Replacing this into Eq. (19) we otain our *final* visiting distribution

$$g_{q_V}(\Delta x_t) = \left(\frac{q_V - 1}{\pi}\right)^{D/2} \frac{\Gamma\left(\frac{1}{q_V-1} + \frac{D-1}{2}\right)}{\Gamma\left(\frac{1}{q_V-1} - \frac{1}{2}\right)} \frac{[T^V_{q_V}(t)]^{-\frac{D}{3-q_V}}}{\left\{1 + (q_V - 1)\frac{(\Delta x_t)^2}{[T^V_{q_V}(t)]^{\frac{2}{3-q_V}}}\right\}^{\frac{1}{q_V-1}+\frac{D-1}{2}}} \ (\forall q_V,\ \forall_D) \tag{21}$$

The second moment of this distribution diverges for $q_V \geq 5/3$, and the distribution becomes not normalizable for $q_V \geq 3$.

There is no particular reason for $T^V_{q_V}$ being equal to $T^A_{q_A}$ but, following [5], we shall use here the simplest choice, i.e., $T^A_{q_A}(t) = T^V_{q_V}(t)$, $\forall t$ (given by Eq. (14)). We can now summarize the whole algorithm for finding a *global* minimum of a given energy/cost function $E(\vec{x})$:

(i) Fix (q_A, q_V). Start, at $t = 1$, with an arbitrary value $\vec{x}_1$ and a high enough value for $T_{q_V}(1)$ (say about 2 times the height of the highest expected "hill"of $E(\vec{x})$, and calculate $E(\vec{x}_1)$;

(ii) Then randomly generate $\vec{x}_{t+1}$ from $\vec{x}_t$ according to Eq. (21) to determine the *size* of the jump Δx_t, and isotropically determine its *direction*;

(iii) Then calculate $E(\vec{x}_{t+1})$:
If $E(\vec{x}_{t+1}) < E(\vec{x}_t)$, replace $\vec{x}_t$ by $\vec{x}_{t+1}$;
If $E(\vec{x}_{t+1}) \geq E(\vec{x}_t)$, run a random number $r \in [0,1]$: if $r > P_{q_A}$ given by Eq. (5) with $T^A_{q_A}(t) = T^V_{q_V}(t)$, retain $\vec{x}_t$; otherwise, replace $\vec{x}_t$ by $\vec{x}_{t+1}$;

(iv) Calculate the new temperature $T^V_{q_V}$ using Eq. (14) and go back to (ii) until the minimum of $E(\vec{x})$ is reached within the desired precision.

3 A SIMPLE D=1 ILLUSTRATION

In this Section we numerically treat a simple $D = 1$ example with a double purpose: on one hand to exhibit how the procedure works and, on the other, to find for which pair (q_V, q_A) the algorithm is the *quickest*. (We recall that $(q_V, q_A) = (1, 1)$ corresponds to CSA and (2,1) to FSA).

We choose the same example treated in [5], namely

$$E(x) = x^4 - 16x^2 + 5x + E_0 \tag{22}$$

where we have introduced the additive constant $E_0 \simeq 78.3323$ so that $E(x) \geq 0$, $\forall x$, thus satisfying the convention adopted below Eq. (5); see Fig. 1. As initial conditions for all of our runs we used $x_1 = 2$ and $T_{q_V} = 100$. In Fig. 2 we can see typical runs for $q_A = 1.1$ and different values of q_V. Clearly the case $q_V = 2.5$ is much faster and precise than classical and fast annealings ($q_V = 1.1 \simeq 1$ and 2 respectively). To study the (q_V, q_A) influence on the quickness of the algorithm we have adopted once for ever, an arbitrary convergence criterium. For each (q_V, q_A) pair we evaluate the mean value of x_t in intervals of 100 time steps. Whenever two successive intervals presented mean values whose difference was smaller than a precision $\varepsilon = 10^3$, we stopped the run. We then evaluated the total iteration time τ and repeated the whole annealing procedure 10 times. Finally, we compute the average total calculation time $< \tau >$. The (q_V, q_A) dependence of the average $< \tau >$ is presented in Fig. 3 for typical values of q_A. Fig. 3 indicates that machines with $q_A = 1.1$ and $q_V = 2.9$ are typically 5 times faster than the Cauchy machine [5], which is in turn about 5 times faster than the Boltzmann machine

[1, 3, 5]. We have done our simulations on a 486 DX microcomputer with a clock of 50 MHz. In this machine each one of the 10 solutions demanded, approximately, 1 minute and 20 seconds of CPU time for $q_V = 2$, and only 20 seconds for $q_V = 2.5$. Finally in Fig. 4 we present the dependence of $< \tau >$ with q_A for $q_V = 2$; for this case the Cauchy machine [5] is the best performant. These results indicate that the quickest algorithm occurs for $q_A = 1$ and $q_V = 3$.

4 CONCLUSION

Inspired in a recent generalization of Boltzmann-Gibbs statistical mechanics, we have heuristically developed a *generalized simulated annealing* (characterized by the parameters (q_V, q_A)) which unifies the so called *classical* (Boltzmann machine; $q_V = q_A = 1$) and *fast* (Cauchy machine; $q_V/2 = q_A = 1$) ones. This computational method is based on stochastics dynamics (which asymptotically becomes, as time runs to infinity, a gradient descent method), and enables, with probability one, the identification of a *global* minimum of any (sufficiently nonsingular) given energy/cost function which depends on a continuous D-dimensional variable $\vec{x}$. While the discrete time t increases, it might happen that $\vec{x}_t$ provisionally stabilizes on a given value, and eventually abandons it running towards the *global* minimum. This temporary residence can be used, as bonus of the present method, to identify *some* of the *local* minima. If sufficiently many computational runs are done by starting at random initial positions $\{\vec{x}_1\}$, this property could in principle be used to identify *all* the *local* minima as well as *all* the *global* ones.

For simplicity, we have mainly discussed herein the restricted region $q_V \geq 1$ and $q_A \geq 1$ (with $E(\vec{x}) \geq 0, \ \forall \vec{x}$), and have identified the $(q_V, q_A) \simeq (2.9, 1)$ machines as the most performant ones in practical terms. This algorithm has been illustrated herein with a simple two-minima $D = 1$ energy function, and has already been successfully used [10] for recovering the global energy minima (with respect to the dihedral angle) of a variety of simple molecules (e.g., $CH_3OH, \ H_2O_2, \ C_2H_6$). It should be very interesting to test the present generalized algorithm with many-body systems presenting a great number of minima (spin-glass-like frustrated systems, traveling salesman problem , neural networks, complex economic systems).

We acknowledge N. Caticha for stressing our attention onto Szu's algorithm [5], as well as K.C. Mundim and A.M.C. de Souza for very useful discussions. At the time of submission of this paper we took notice that this algorithm (informally communicated by us to a few people) has already been succesfully implemented for the Traveling Salesman Problem [11, 12], for fitting curves [13, 14], and for a problem of genetic mutations [15].

Caption for figures

Fig. 1: $D = 1$ energy function $E(x) = x^4 - 16x^2 + 5x + E_0$ vs. x for $E_0 = 78.3323$; global minimum $x_1^* = -2.90353$ and $E(x_1^*) = 0$; maximum: $x_2^* = 0.156731$ and $E(x_2^*) = 78.7235$; local minimum: $x_3^* = 2.74680$ and $E(x_3^*) = 28.2735$.

Fig. 2: Typical runs of the GSA algorithm x_t vs. t (annealing time) for initial conditions $x_1 = 2$, $T_{q_V}(1) = 100$. All four runs correspond to $q_A = 1.1$; a) $q_V = 1.1$, b) $q_V = 1.5$, c) $q_V = 2$, d) $q_V = 2.5$. Notice the different scales for the ordinates.

Fig. 3: Average total calculating time $< \tau >$ vs. q_V for two typical values of q_A ($\triangle$: $q_A = 1.5$; $\odot$: $q_A = 1.1$).

Fig. 4: Average total calculation time $< \tau >$ vs. q_A for $q_V = 2$.

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